1 The Maximum likelihood target function

In order to be consistent in notation, I will, try to derive a liklelihood target function for the usual case, and use this knwoledge to figure out the exact meaning of α and β used in phenix.refine.

$$p(\mathbf{F}_{\mathbf{H}_o}, \mathbf{F}_{\mathbf{H}_c}) = N([\mu_o, \mu_c], \Sigma) \tag{1}$$

As this distribution has jot yet been conditioned, the mean values are equal to zero. The variance covariance matrix can be written as

$$\Sigma = \begin{pmatrix} \mathbb{E}[\mathbf{F}_{\mathbf{H}_o}\mathbf{F}^*_{\mathbf{H}_o}] & \mathbb{E}[\mathbf{F}_{\mathbf{H}_c}\mathbf{F}^*_{\mathbf{H}_o}] \\ \mathbb{E}[\mathbf{F}_{\mathbf{H}_o}\mathbf{F}^*_{\mathbf{H}_c}] & \mathbb{E}[\mathbf{F}_{\mathbf{H}_c}\mathbf{F}^*_{\mathbf{H}_c}] \end{pmatrix} \tag{2}$$

Specificy the elements of the variance co-variance matrix:

$$\Sigma = \begin{pmatrix} \sigma_p & D_p D_c \sigma_p \\ D_p D_c \sigma_p & D_c \sigma_p \end{pmatrix} \tag{3}$$

D_p models the effect of positional parameters, whereas as D_c models the effect of the completeness of the model.

Result 4.6 of Johnson and Wichern states that the mean of a conditioned multivariate Gaussian is equal to

$$\mu_{new} = \mu_1 + \mathbf{\Sigma}_{12}\mathbf{\Sigma}_{22}(\mathbf{x}_2 - \mu_2) \tag{4}$$

The conditioned variance covariance matrix is equal to

$$\mathbf{\Sigma}_{new} = \mathbf{\Sigma}_{11} - \mathbf{\Sigma}_{12}\mathbf{\Sigma}_{22}^{-1}\mathbf{\Sigma}_{21} \tag{5}$$

For our case refinement case, specify the elements:

$$\begin{aligned} \Sigma_{11} &= \sigma_p & (6) \\ \Sigma_{12} &= D_p D_c \sigma_p & (7) \\ \Sigma_{21} &= D_p D_c \sigma_p & (8) \\ \Sigma_{22} &= D_c \sigma_p & (9) \end{aligned}$$

And thus,

$$p(\mathbf{F}_{\mathbf{H}_o} | \mathbf{F}_{\mathbf{H}_c}) = N\left[D_p \mathbf{F}_{\mathbf{H}_c}, (1 - D_p^2 D_c)\sigma_p\right] \tag{10}$$

Spelling it out:

$$p(\mathbf{F}_{\mathbf{H}_o}|\mathbf{F}_{\mathbf{H}_c}) = \frac{1}{\pi(1-D_p^2 D_c)\sigma_p} \times \exp\left[(\mathbf{F}_{\mathbf{H}_o} - D_p\mathbf{F}_{\mathbf{H}_c})^* (1-D_p^2 D_c)^{-1}\sigma_p^{-1} (\mathbf{F}_{\mathbf{H}_o} - D_p\mathbf{F}_{\mathbf{H}_c})\right]$$

The quadratic form in the exponent is equal to

$$Q = |\mathbf{F}_{\mathbf{H}_o}|^2 - D_p|\mathbf{F}_{\mathbf{H}_c}|^2 - 2D_p|\mathbf{F}_{\mathbf{H}_o}||\mathbf{F}_{\mathbf{H}_c}|\cos(\phi_c - \phi_o) \tag{11}$$

Putting things together, this brings

$$\begin{aligned} p(\mathbf{F}_{\mathbf{H}_o}|\mathbf{F}_{\mathbf{H}_c}) &= \frac{|\mathbf{F}_{\mathbf{H}_o}|}{[2\pi(1-D_p^2 D_c)\sigma_p]^{1/2}} \times \\ &\exp\left[\frac{|\mathbf{F}_{\mathbf{H}_o}|^2 - D_p|\mathbf{F}_{\mathbf{H}_c}|^2}{(1-D_p^2 D_c)\sigma_p}\right] \times \\ &\exp\left[-\frac{2D_p|\mathbf{F}_{\mathbf{H}_o}||\mathbf{F}_{\mathbf{H}_c}|\cos(\phi_c - \phi_o)}{(1-D_p^2 D_c)\sigma_p}\right] \end{aligned} \tag{12}$$

Integrate out ϕ_o

$$\begin{aligned} p(|\mathbf{F}_{\mathbf{H}_o}|||\mathbf{F}_{\mathbf{H}_c}|, \phi_c) &= \frac{2|\mathbf{F}_{\mathbf{H}_o}|}{(1-D_p^2 D_c)\sigma_p} \times \\ &\exp\left[\frac{|\mathbf{F}_{\mathbf{H}_o}|^2 - D_p|\mathbf{F}_{\mathbf{H}_c}|^2}{(1-D_p^2 D_c)\sigma_p}\right] \times \\ &I_0\left[\frac{2D_p|\mathbf{F}_{\mathbf{H}_o}||\mathbf{F}_{\mathbf{H}_c}|}{(1-D_p^2 D_c)\sigma_p}\right] \end{aligned} \tag{13}$$

If this is compared to the definition of σ_A as given in Murshudov's et al, Refmac paper, one quickly sees that

$$D_p^2 D_c = \sigma_A^2 \tag{14}$$

$$D_p = D \tag{15}$$

Inspecting Afonin et al, One can see that

$$\alpha = D_p \tag{16}$$

$$\beta = (1-D_p^2 D_c)\sigma_p \tag{17}$$